3.2 Combustion and Energetic Materials

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Overview

Combustion of solid propellant composed of energetic materials is the driving thermomechanical force in the operation of a solid rocket motor. Accurate modeling and simulation of the combustion and resulting regression of solid propellants entails research activities in several areas, including the description and propagation of the propellant combustion interface, modeling of solid propellant flames, combustion instability analysis, and constitutive modeling of energetic materials.

The Combustion and Energetic Materials (CEM) group has a hierarchical strategy for developing solid propellant combustion models based on incremental physical/modeling complexity and parallel experimental validation. Under this strategy the daunting complexity of composite solid propellant combustion is attacked by isolating various physical/chemical phenomena within a lowest dimensional model necessary to address each level. Non-aluminized propellant issues are tackled first and then aluminum is added.

Simulation and Validation

Three-Dimensional Propellant Combustion Simulation (Buckmaster, Jackson, Massa, Wang, Cui)

The research group of Jackson, Buckmaster, Massa and Wang has been engaged for a number of years in the numerical simulation of three-dimensional heterogeneous solid propellant combustion. To this end we have, for the first time, created a three dimensional code that fully couples the propellant solid physics with the gas-phase combustion in a non-planar non-steadily regressing propellant surface. We have validated burning rate predictions and the variations of these rates with propellant morphology by comparisons with experiment, without the use of curve fitting with three-dimensional results. We have, for the first time, been able to examine numerically the impact of acoustic waves on a burning heterogeneous propellant, and describe the properties of the reflected wave, a crucial issue in rocket chamber stability. Furthermore, we have, for the first time, been able to describe the proper injection boundary conditions for LES simulations, necessary for meaningful solid rocket motor simulations. For aluminized propellants we have developed algorithms that accurately predict the statistics of the aluminum agglomerates that form on the surface and which, after detachment, are of great concern to the rocket industry because of their impact on the nozzle. Aluminum agglomeration in the throat seriously degrades the specific impulse of the motor

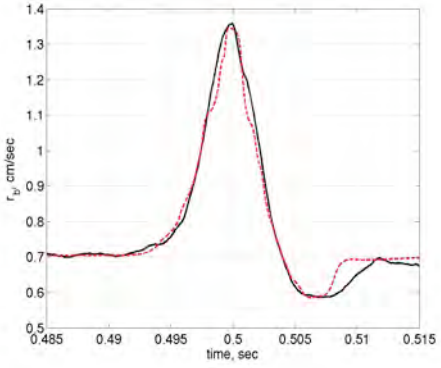

Fig. 3.2.1: Burn rate as function of time for pressure pulse. Results from *Rational_Rocburn* (red) compare well with multidimensional results from *Rocfire* (black).

and hence significantly shortens the operational range of a motor. Hence this work has an enormous potential in that by tailoring the characteristics of the propellant packs to minimize aluminum agglomeration, one may be able to extend operating range of Air Force strategic missiles.

A number of important projects have been worked on in the previous year, and are summarized below. These projects include the completion or modification of previous work, as well as the beginnings of new projects.

P1. *Rational Rocburn* We have developed what we call *Rational_Rocburn*, a *Rocburn* module that is constructed by spatial averaging of *Rocfire*, accounting for unsteady effects on the propellant time scale (see Figure 3.2.1). A key component of this module is a look-up table that properly accounts for the heat flux to the propellant surface from the *Rocfire* combustion field. This module has been incorporated into *Rocstar* and the central goal of the CEM group has now been achieved, albeit for non-aluminized propellants. Last year we published results for two-dimensional packs. We are currently extending the analysis to three-dimensional packs, and expect to finish the project before the end of the current fiscal year.

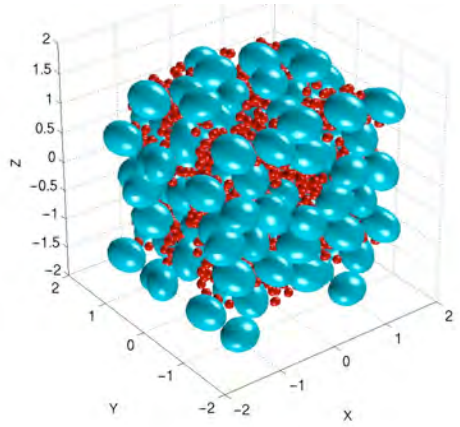

Fig. 3.2.2: Three-dimensional bimodal pack of ellipsoids generated using *Rocpack*.

P2. *Rocpack* In order to simulate the combustion of three-dimensional composite propellants, a representation of the solid is required. To this end we previously developed *Rocpack*, a dynamic packing algorithm that takes as input industrial data size distributions, and generates a representative "virtual" solid propellant with the same volume fraction as that used in industry. The original version of the code only packed AP particles, and was not user friendly. We therefore extended the code this past fiscal year to include a number of important features.

The particles can now be AP, HMX, RDX, aluminum, etc., or a combination, embedded in a binder, usually taken to be HTPB. The current version of the code is written in Fortran 90 and uses MPI. It has a user-friendly interface so that non-technical people can use the code. This new interface is called *Rocprepack*. *Rocprepack* and *Rocpack* are both in a CVS directory for others to download.

In the mixing process of real propellants, large AP particles are mixed first so that the binder coats each AP particle; smaller AP particles are then poured into this mixture. This generates a pack where the binder separates the large AP particles. To better simulate this process, we have added a "coating" parameter to Rocpack, which allows the user to define an averaged separation distance for all particles. A typical coating value might be 190 nm.

Typical packs range in size from as few as 30,000 particles, which can be generated on 16-processors in about one day, up to 500,000 particles, which requires 100-processors and takes approximately 36 wall clock hours to generate. Both ATK/Thiokol and Aerojet West have expressed interest in using this code in their Air Force sponsored research, and it is our intent to license the code to them. In the coming fiscal year we plan to make *Rocprepack* a GUI driven interface.

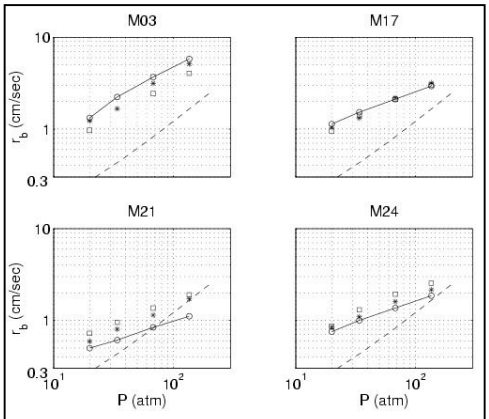

Fig. 3.2.3: Plot of burn rate as function of pressure for four different Miller packs. Experiments – circles; 2 step kinetics – box; 3 step kinetics – asterisks; pure AP burn rate curve – dashed line.

In addition to the modifications listed above, the inclusion of non-spherical particles, in particular ellipsoids, was added as a new feature. Figure 3.1.2 shows a random pack of bimodal ellipsoidal particles. The capability to model non-spherical particles was added to study the effect of particle shape on burn rates. Combustion results using *Rocfire* show that if the ellipsoids are randomly oriented, then the average burn rate differs little from their spherical counterparts. However, if the ellipsoids are aligned in some preferred direction, then the average burn rate can be changed significantly. This might have practical implications in motor design, but we plan no further modifications unless asked by the rocket industry.

P3. *Rocfire* – Non-aluminized Once the "virtual" propellants have been built, they need to be "virtually burned". To this end we have previously developed Rocfire: in the gas phase this solves the three-dimensional zero Mach number equations for a reacting gas, and in the solid phase solves the three-dimensional unsteady heat equation. The solid and gas are closely coupled using appropriate jump conditions and pyrolysis laws across their interface, which is represented using level sets, hereby allowing the surface to take on any shape the physics dictates. The code is written in Fortran 90 and uses MPI, and uses GMRES to speed up the pressure solver. Typical grid sizes are approximately 1-10 microns, while the packs are on the size of 1-2 millimeters. Our experience is that this size is sufficient for purposes of gathering statistics. To get the necessary statistics, typical run time is approximately 2-3 days using 100 processors for a fixed pressure. To get a complete pressure history, the code needs to run for several weeks given dedicated computer time. A variation of Rocfire (non-aluminized) has been developed using a three-step kinetics model rather than a two-step model as in the first implementation. Superior agreement with experimental burning rates of various Miller packs is achieved (see Figure 3.2.3) and further improvement in this respect cannot be expected. The new model leads to intrinsic instabilities under some circumstances, the stability boundaries of which cannot be expected to match reality, but there might be no resolution of this difficulty within the framework of global kinetics. We hope to revisit this difficulty in the coming fiscal year using the newly developed code *Rocfit*, as described below.

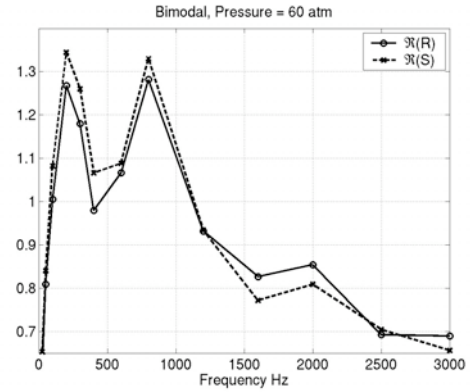

Fig. 3.2.4: Mass-flux respose function (R) and velocity response function (S) as function of frequency for bimodal pack. Note that the response functions have multiple peaks.

P4. Acoustics *Rocfire* has been applied to an important physical problem, namely the burning response to an impinging acoustic wave. There are serious rocket stability issues should the reflected wave have a larger amplitude than the incident wave. We have been able to compare the mass-flux response function and the velocity response function (both functions of frequency) and have shown to what extent they differ (see Figure 3.2.4). Since the velocity response cannot be measure experimentally, whereas the mass-flux response can, it is always assumed that they are equal in making stability predictions, and we have described the errors that can arise in doing this. The original work was for two-dimensional packs, but we hope to revisit the problem in three-dimensions within the coming fiscal year.

P5. *Rocfit* The use of detailed kinetic schemes is still too computationally intensive for three-dimensional simulations so global kinetic schemes are employed instead. However, global kinetic schemes involve a number of parameters that must be chosen in a rational way. To this end we have recently developed *Rocfit*, a numerical software tool that uses a numerical optimization scheme based on genetic algorithms to choose optimal parameters. *Rocfit* runs on an MPI platform using 100-

processors, and takes about 12 hours to generate a set of parameters. *Rocfit* is currently being used to calibrate the global kinetic parameters for HMX/HTPB propellants for which extensive experimental data are available. Figure 3.2.5 shows an instantaneous temperature profile for one HMX propellant pack. In the near future we will use *Rocfit* to re-calibrate the AP/HTPB kinetic parameters, and compare burn rate results with previous work. It is expected that by using *Rocfit*, the intrinsic instability mentioned earlier when using hand optimization, can be avoided.

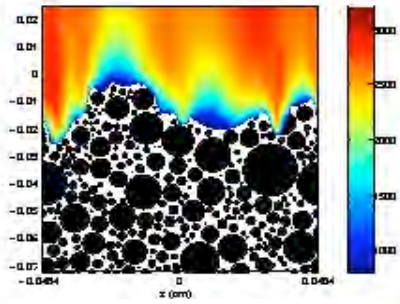

Fig. 3.2.5: Instantaneous temperature contours for HMX/HTPB propellant; slice through three-dimensional pack.

P6. Far-field Solutions The CSAR code *Rocstar* accommodates turbulence using large-eddy simulations. Here a new challenge, not present in traditional scenarios, is a proper accounting of the nature of the injected flow at the chamber/propellant boundary. Particularly for heterogeneous propellants, this flow and the vorticity it carries is neither steady nor spatially uniform. These fluctuations could well have an effect on the overall chamber flow and, indeed, there is a significant amount of experimental and computational work that demonstrates the effect of perturbations of initial or boundary conditions on the long-time or far-field solution of turbulent flow-fields. Of particular interest in rocket flows is the interaction between the omnipresent acoustic waves and fluctuations of the injected flow, and a number of studies have shown how important this can be for certain parameter values. For these reasons alone, notwithstanding the significance of any findings, it is of interest to describe the nature of the flow-field at an intermediate distance above the propellant surface, intermediate in the sense that the distance is large compared to the scale of the flame structure, but small compared to appropriately defined flow scales. To this end the far-field of *Rocfire* (~ 1mm from the surface) is currently being examined for very large packs in an attempt to characterize the flow field fluctuations that should be used as boundary conditions for the LES simulations of the Fluids Group. Preliminary work has been carried out and implemented into *Rocstar*. Figure 3.2.6 shows the most recent work. The combustion field beyond the flame zone has large velocity and temperature fluctuations (see Figure 3.2.6, left panel), and these fluctuations can influence the head end pressure (see Figure 3.2.6, right panel). We note that different propellant morphologies yield different head end pressure fluctuations, an observation impossible with traditional treatment of the propellant surface. We will continue this work in the

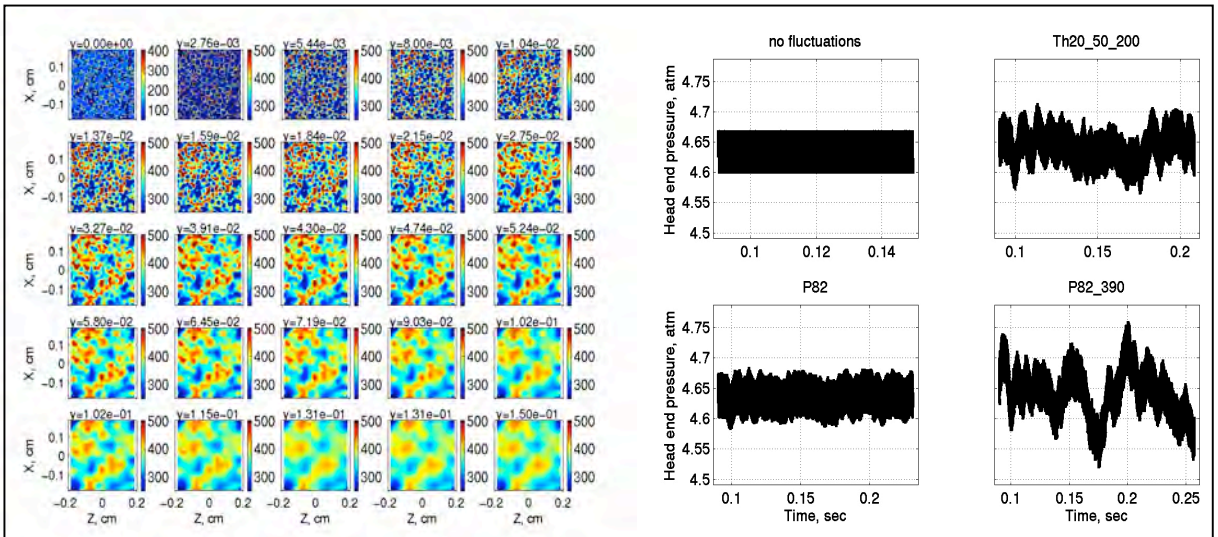

Fig. 3.2.6: Left: Instantaneous velocity contours (33% fluctuations) as function of normal distance above propellant surface; similar contours are obtained for temperature field (14% fluctuations about mean). Right: Head end pressure as function of time for four different mass flux input distributions.

coming fiscal year. This work is done in collaboration with F. Najjar.

P7. *Rocfire* – Aluminized The *Rocfire* version of the code described previously does not take into account aluminum. Since almost all solid propellants of interest contain some amount of aluminum, the code is being extended to include the necessary particle tracking and physics modules. The propellant surface and aluminum particles in the gas phase are tracked using level sets. Although the code is not complete, benchmark studies indicate that it will take several weeks on 100 processors for a single successful run. Figure 3.2.7 shows instantaneous combustion fields for a two-dimensional pack, the aluminum particles being colored in copper. Figure 3.2.8 shows the instantaneous temperature surface field for a three-dimensional pack. The aluminum particles are obvious, and are colored according to the temperature field it locally sees. This project is an enormous one, and because of its significance to the rocket industry, will be continued in the coming fiscal year.

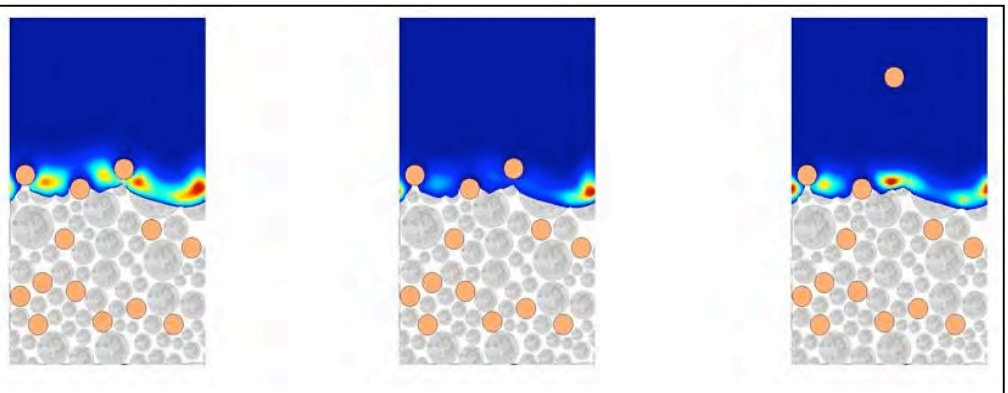

Fig. 3.2.7: Results from 2D aluminum *Rocfire* code. Aluminum (shown in copper) is initially embedded within propellant. As propellant surface regresses due to burning, aluminum particle becomes exposed to hot gases, detaches, and then moves away from surface. Surface regression, detachment and subsequent evolution of aluminum particles, are handled using level sets.

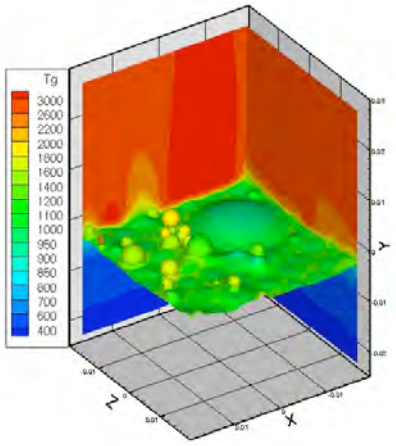

Fig. 3.2.8: Instantaneous surface temperature field. Small particles are aluminum and particle in farthest corner is large 200-micron AP particle. Aluminum particles near surface are colored according to local temperature experienced. Surface regression, detachment and subsequent evolution of aluminum particles are handled using level sets.

P8. Agglomeration Modeling Here we discuss recent work on aluminum agglomeration, an important subject currently under investigation by both ATK/Thiokol and Aerojet. Typical solid rocket motor propellants, such as those used in the space shuttle boosters, are composed of ammonium perchlorate (AP) and aluminum (Al) particles embedded in fuel binder. A typical composition, by weight, is 71% AP, 18% Al, and 11% binder. The aluminum reacts exothermically with H2O and CO2 in the chamber, increasing the specific impulse by approximately 10%. It also provides efficient damping of chamber instabilities, a desirable effect. However, there are undesirable effects such as slag accumulation, nozzle erosion, and significant exhaust signatures. Because of these, aluminum behavior is one of the most important problems faced by the solid propellant industry. An essential feature is agglomeration of particles at the propellant surface. To this end we have developed an agglomeration model, based on Rocpack (see Figure 3.2.9, left panel), which yields both the agglomeration diameter and the agglomeration distribution (see Figure 3.2.9, right panel), which are critical for meaningful simulations of nozzle and plume flows. The agglomeration model has recently been

applied to a number of IHPRPT propellants developed at Aerojet West, and the results are extremely encouraging (see Figure 3.2.9, right panel). The funding for Aerojet comes from the propulsion group at Edwards Air Force Base AFRL/PRS. We plan to further improve the agglomeration model in the coming fiscal year, and apply it all the data we can obtain from Aerojet and ATK Thiokol.

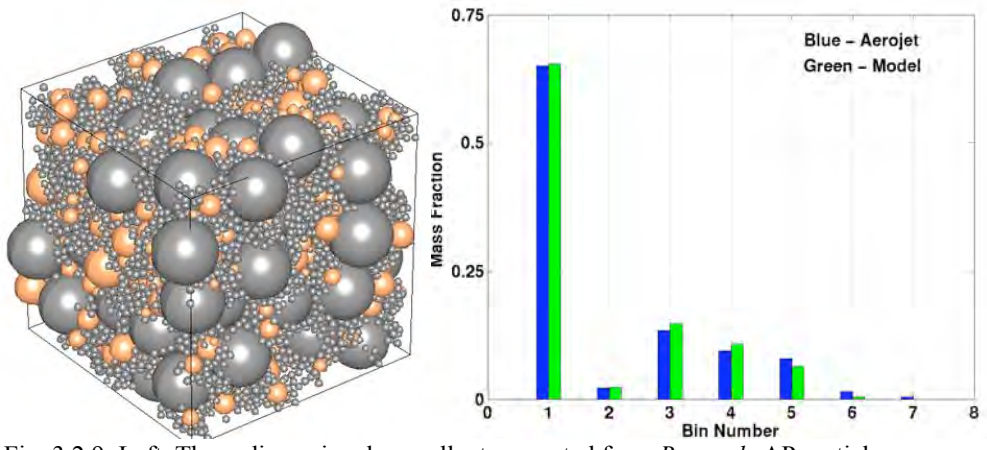

Fig. 3.2.9: Left. Three-dimensional propellant generated from *Rocpack*. AP particles are shown in gray, aluminum particles shown in copper. Right. Results from agglomeration model comparing agglomeration distribution from experiments (blue, from Aerojet) with that of CSAR model (green). Agreement between model and experiments is excellent.

P9. Radiation Modeling for Fine Aluminum Modern propellants are composed of a combination of oxidizer (usually AP) with aluminum. The aluminum particles added to propellants can vary widely in size, and recently there has been a significant interest in ultra-fine aluminum (Alex) with particles of order 10-100 nanometers in diameter. We are interested in propellants that contain Alex and conventionally size aluminum (~20 micron diameter), and the computational domains of interest are typically 1 mm in size. Then the conventional particles can be numerically resolved, but the small ones cannot. Thus, to account for the small particles, it is necessary to homogenize them into the binder, to assume that the binder and the small aluminum particles are constituents of a homogeneous blend. To this end we have recently constructed a model for the blend that takes into account radiation. The experimental results reported by Dokhan, et al. (2003) are used for calibration and comparison. Figure 3.2.10 shows the burn rate as a function of pressure for three different aluminum loadings. Note that our model compares well with the experimental data. This work is currently being extended to three-dimensional packs with fine aluminum. Radiation equations have been written down and will be implemented into Rocfire in the coming fiscal year, along with comparisons to existing AP based experimental data.

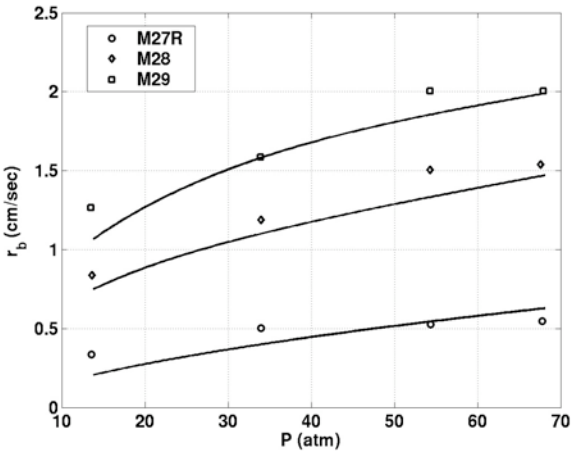

Fig. 3.2.10: Comparisons of burn rate as function of pressure between the model (solid lines) and experimental data (circles) of Dokhan, et al. 2003.

Project Plans A number of combustion projects critical to the overall success of *Rocstar* as a predictive tool for solid rocket motor simulations will continue in the coming fiscal year. The integration of *Rational_Rocburn* into *Rocstar* has recently been completed, and attempts will be made to develop a similar module for three-dimensional packs and for aluminized propellants. *Rocpack* is essentially complete, although we will build a GUI for the

interface package *Rocprepack*. Modifications to *Rocpack* to include the packing of three-dimensional elliptic cylinders might be considered if enough interest exists. The development of *Rocfit* is complete, and the coming fiscal year will see this important tool being applied to AP/HTPB propellants as well as more modern propellants of interest. Acoustics is an important problem, and if time allows we hope to revisit this problem for a more in-depth analysis, and to make it a module of *Rocstar*. The work on proper injection boundary conditions for meaningful LES simulations will continue to be an important problem. A module for stochastic injection boundary conditions was incorporated *into* Rocstar last fiscal year, and we expect further improvements in the coming fiscal year. Work on aluminized *Rocfire* will continue, the goal there being a fully functional three-dimensional version. We believe that one of the most important contributions that can be made here is to the agglomeration problem, one of enormous interest to the US industry and of at least equal value to any *Rocstar* application. We are also examining the role of Alex (nanometer scale aluminum) in the combustion process, as there is considerable interest in this in the industry. The aluminum work and related issues (such as melt layers) could easily extend to the end of the current contract period, but we expect that interim results within the next year framework will be of fundamental value to the integrated code.

Combustion in Propellant Cracks (Short and Kessler)

Kessler and Short have been performing very high resolution simulations of flow in a slender channel with side-wall injection using a sixth-order compact finite difference scheme as part of a validation and verification process of an on-going Rocstar simulation of reactive burning inside a thin propellant crack (25-100 microns wide). Combustion in cracks is an important issue for stable rocket motor performance and in the behavior of energetic materials under damage. The current calculations are performed in a sufficiently long crack (40mm) such that chocking flow conditions occur during the burn. A range of combustion behaviors are observed, including stable and oscillatory burning.

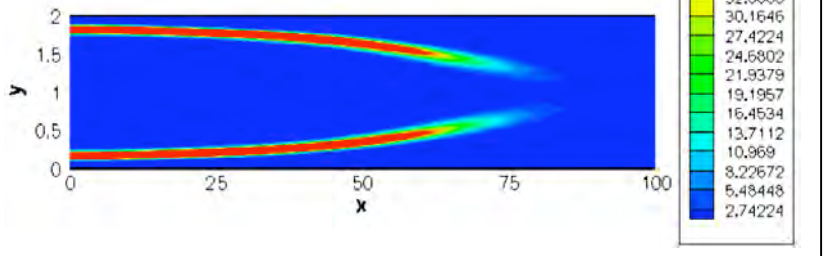

Fig. 3.2.11: Reaction rate profiles are simulated for combustion in thin propellant cracks.

Figure 3.2.11 shows a snapshot of the reaction rate profiles during the oscillatory burning of a flame in the channel for a low Reynolds number case. Quenching of the flame occurs near the sonic flow surface. Comparisons between the Rocstar calculations on the burning inside a propellant crack will be made with the high-order calculations to ascertain the ability to the *Rocstar* code to capture acoustic-viscous-reaction interactions on-going inside the crack.

The second project involves the use of *Rocstar* to stimulate the flame structure inside a sub-millimeter scale microburner that has been developed at UIUC by Profs. Masel and Shannon as part of a DARPA/MURI program on the development of micro-scale fuel cell technology. The development of microburner technology is currently being explored for use in areas such as power sources for micro-mechanical systems (micro-engines), as heat sources for micro-fuel convertors, and for portable chemical/biological detectors.

As the microburners are reduced in size, heat losses to and transfer along the burner walls become dominant, and some unusual flame cells are observed which have an adverse effect on microburner efficiency. For example, in the UIUC burners the laminar flame is seen to break up into flame cells, structures which have also been attributed to the failure of a micro-scale Wankel Engine developed at

Berkeley. Figure 3.2.12 shows a schematic of the UIUC microburner geometry, and an image of the flame cells looking down from the top of the burner. *Rocstar* is being used to stimulate and understand the physics behind the formation of the three-dimensional flame cells, with the aim that microburner efficiency can be improved. Thus far, Kessler has explored how to set up the microburner geometry within Rocstar, and calculations will be undertaken in the next year.

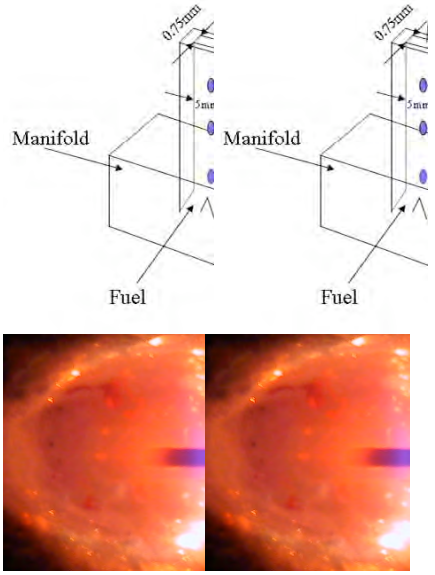

Fig. 3.2.12: Microburner geometry and resulting flame cell simulations for micro-scale Wankel engine.

During the upcoming year, we will concentrate extensively on the use of the integrated CSAR code for the analysis of flame structure in the three-dimensional microburner geometry. Specific plans include working with Andreas Haselbacher and Luca Massa to add reduced chemistry combustion for methane/air and propane/air to the current reactive version of *Rocflu*. Potentially, we may be able to add full reaction chemistry via the integration of Chemkin into *Rocflu*. Also, variable conductivity heat conduction for alumina and silica need to be added to *Rocsolid*. The integrated code will then be used to understand the physics behind the formation of 3D cellular flames in the microburner, as well as determining the typical conversion rate of fuel to ascertain the effectiveness of the microburner in supplying heat to a micro-fuel-reformer in a fuel cell configuration. In addition to this study, we will be conducting further detailed comparisons between the predictions of the integrated code and that of the high-order compact scheme for the problem of flame propagation in a micro-crack in order to ascertain the relative accuracy of the integrated code.

Quantum Monte Carlo Simulations of Hot, Dense Matter (Ceperley and Esler)

We have further developed, tested and applied to dense hydrogen, better methods for *ab initio* simulation including novel forms for the wavefunction and methods for sampling electronic configurations more efficiently. We performed simulations of molecular and metallic hydrogen in the temperature range of 300-1000K without assuming an intermolecular potential or a density functional for the electrons and including effects of proton zero-point motion and found values for the melting temperature of solid hydrogen at high pressures. We have found the simulations using density functional theory melt at too low temperatures and overemphasize the sharpness of the molecular to atomic transition. We have developed and tested a new method to compute forces and energy differences using quantum Monte Carlo and made the first such calculations on polyatomic molecules with higher accuracy than with any other method. We have developed a new method and codes to eliminate core electrons and have tested these pseudopotentials on several atoms and molecules. We have further developed an object oriented code in C++ to perform Path Integral Monte Carlo using these pseudopotentials and have tested this on sodium.

Combustion Validation using 2-D Laminate Propellants (Brewster, Fitzgerald, and Mullen)

This project uses AP/HTPB 2-D laminate propellants with UV/IR imaging spectroscopy to obtain data for validation of heterogeneous solid propellant combustion models. The non-aluminized phase of this work was completed this year with the graduation and PhD dissertation of Russ Fitzgerald. The aluminized phase of the work was begun with the PhD project of Jessica Mullen.

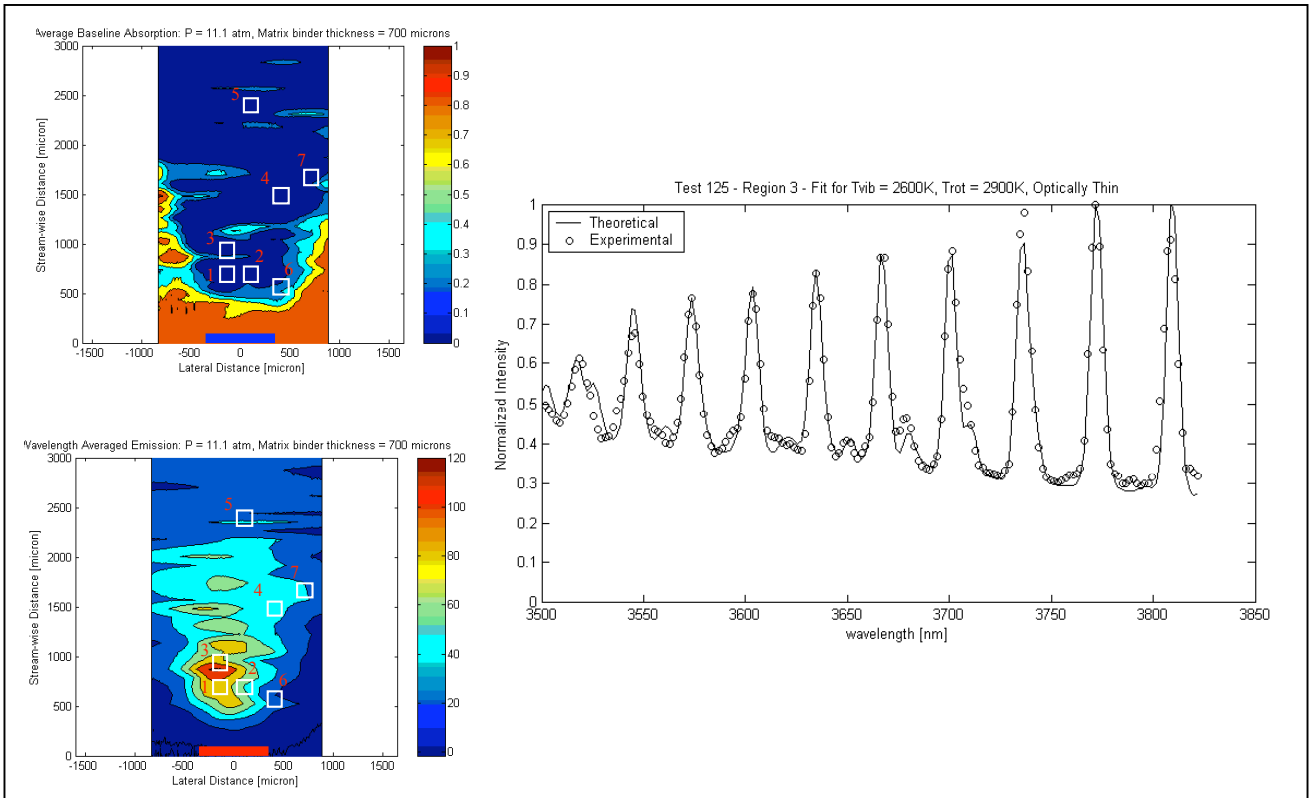

Fig. 3.2.13: HCl vibrational/rotational temperature from emission imaging spectroscopy in AP/HTPB laminate propellant flame

The non-aluminized results obtained during the last year included HCl rotation-vibrational temperature measurements from IR absorption and emission imaging spectroscopy. These results are the first of their kind reported for heterogeneous solid propellants. Figure 1 shows an example of results using emission imaging. The vibrational-rotational band structure can be seen in the figure on the right. The experimental data points are well fit by an optically thin spectroscopic model for rotational and vibrational temperatures of 2900 K and 2600 K, respectively. The flame images on the left show the spatial region in the flame from where the temperature spectrum on the right was obtained. The top image on the left is average baseline absorption and the bottom left figure is wavelength-averaged emission. These results are representative of many that were obtained for various pressures and fuel-layer thicknesses. These data give detailed, spatially resolved flame temperature and indicate the possibility of non-equilibrium. The results provide a wealth of data for comparison with and validation of heterogeneous solid propellant combustion models.

The next phase of this project using aluminized laminates was begun this year. Aluminum agglomeration behavior is an important feature of composite solid propellant combustion. It strongly influences motor performance and it is strongly influenced by the flame structure of the AP/binder components that was studied in the preceding phase of this work. Current combustion modeling efforts in CSAR are focusing on aluminum agglomeration behavior; again validation data is needed. This work will supply some of that data and do so with a unique, first of its kind, approach. The same laminates used previously are being loaded with aluminum powder and their combustion observed to obtain data on agglomeration behavior, such as agglomerate size. This project will run the duration of the lifetime of the center.

Full Burnout Simulation: 3-D Grain Evolution and Internal Ballistics (Tang, Brewster, Kuznetsov, Willcox, and Stewart)

The ultimate goal of this project is to simulate the full burnout of a large-scale SRM, such as the 120 seconds of RSRM operation, including ignition transients, quasi-steady burnback, and tail-off using simplified physical models to reduce computational requirements. One of the key points in solid rocket motor performance analysis is the mass injection into the motor resulting from the combustion of solid propellant. In simulating mass flux into the internal port volume, it is crucial to determine the burning surface area and 3D description is a must. We have developed a fast computational method (*Rocgrain*) for simulating the evolution of the burning surface of a complex, three-dimensional solid rocket motor propellant grain using a signed minimum distance function (MDF). By integrating *Rocgrain* with a simplified flow solver and combustion modes including erosive burning and unsteady nonlinear dynamic burning corresponding to transient energy storage in the heated surface layer of the propellant, *Rocballist* is developed to simulate the internal ballistics of solid rocket motors.

Solid Propellant Grain Design and Burnback Simulation using a Minimum Distance Function
Rocgrain has been developed in collaboration with M. A. Willcox, Professor M. Q. Brewster, and Professor D. S. Stewart. The resulting code (*Rocgrain*) allows motor grain design by user-friendly commercial computer-aided-design (CAD) programs. The MDF is calculated using stereolithography surface information from the CAD file and propellant surface burnback is simulated by manipulation of the initial MDF. Figure 3.2.14 depicts the initial grain geometry of the Naval Air Warfare Center (NAWC) tactical motor #6 with star-aft configuration drafted by Pro-E. A full motor burn simulation of the time evolution of Motor #6 propellant surface (at a constant burning rate of 1.0 cm/s) using *Rocgrain* is shown in Figure 3.1.15. Motor #6 is a full-length star-aft grain design that has end-burning sections, variable cross-section star patterns, inhibited surfaces, and burning surface contacting the insulation/case at various times. Results indicate *Rocgrain* to give adequate accuracy with acceptable computation time for time scales of the full motor burn. This enables a single geometric tool to be used for describing the propellant grain geometry for both grain design and internal flowfield analysis.

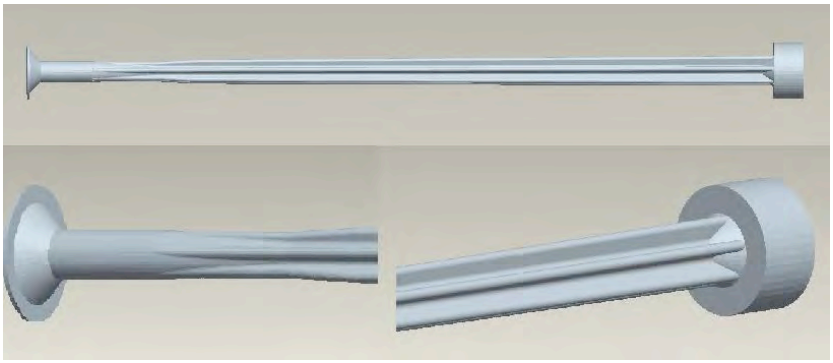

Fig. 3.2.14: Pro-E Screen Capture – NAWC Motor #6

Solid Rocket Motor Internal Ballistics Simulation using Three Dimensional Grain Burnback
Rocballist has been developed in collaboration with M. A. Willcox, Professor M. Q. Brewster, Professor D. S. Stewart, and Dr. I. R. Kuznetsov). Internal ballistics simulations of solid rocket motors using *Rocballist* have been conducted with the propellant grain's three-dimensional burning surface geometry described by a new minimum distance function approach (*Rocgrain*) and the internal flowfield represented by one-dimensional, time-dependent, single-phase compressible flow equations. The combustion model includes erosive burning and unsteady nonlinear dynamic burning. Figure 3.1.15 shows the internal ballistics calculations of NAWC Motor #6 with and without erosive burning. Results show a much improved prediction of the initial pressure trend with the addition of erosive burning. The results also show that with sufficiently accurate models of dynamic burning and erosive burning, it is reasonable to expect reliable internal ballistics predictions with suitable simplified flow-

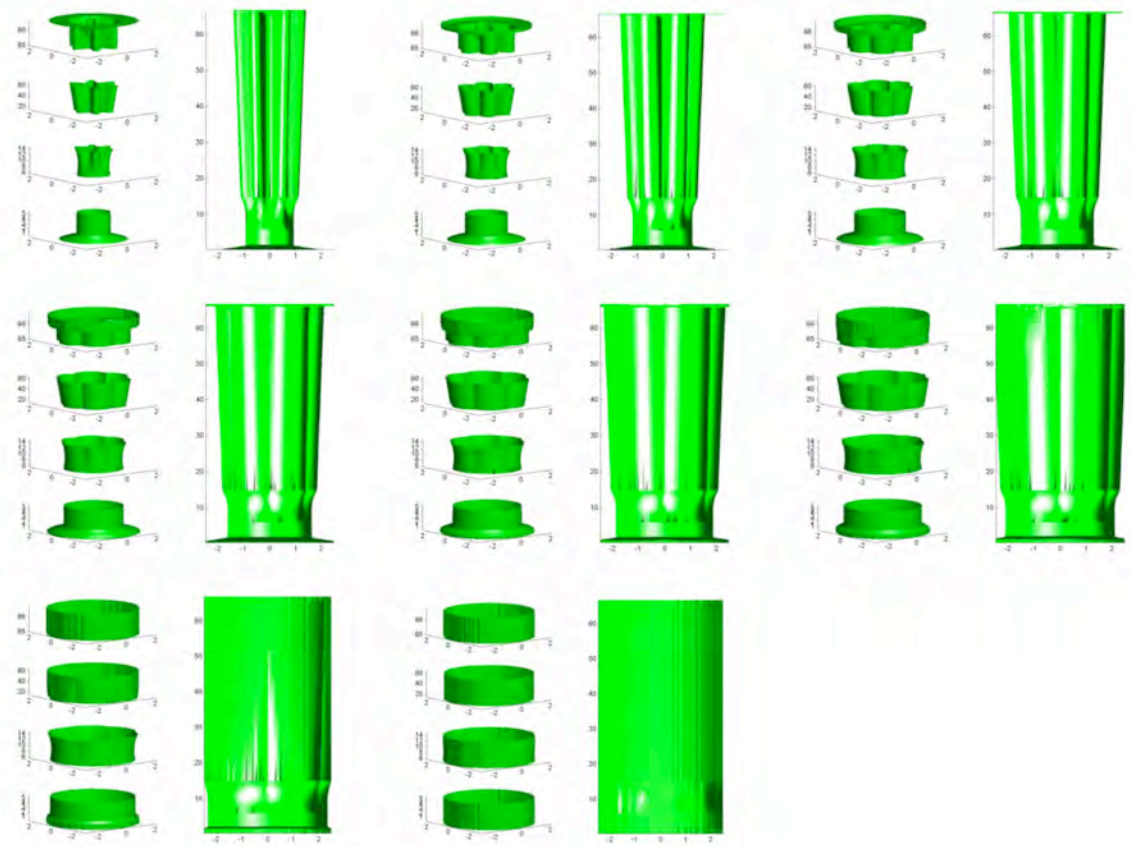

Fig. 3.2.15: Motor #6 surface profiles at sequential times (0.0, 0.6, 1.2, 1.8, 2.4, 3.0, 3.6, and 4.4 s).

field models, thereby realizing significant reductions in computation time compared with three-dimensional, multi-phase reacting flow simulations.

Future Plans Development of *Rocgrain* and *Rocballist* will be focused on RSRM full history (120 seconds) simulation. The necessary tasks include (1) implementation of subcomponents such as ignition and erosive burning models, (2) validation of the numerical results by comparing with available measured tactical motor data, and (3) conversion of current RSRM Pro/E model to the input format required by *Rocgrain.* Upon successful RSRM 120-second full burn simulation using *Rocgrain*/*Rocballist*, integration of *Rocgrain/Rocballist* with the integrated system code *Rocstar* will

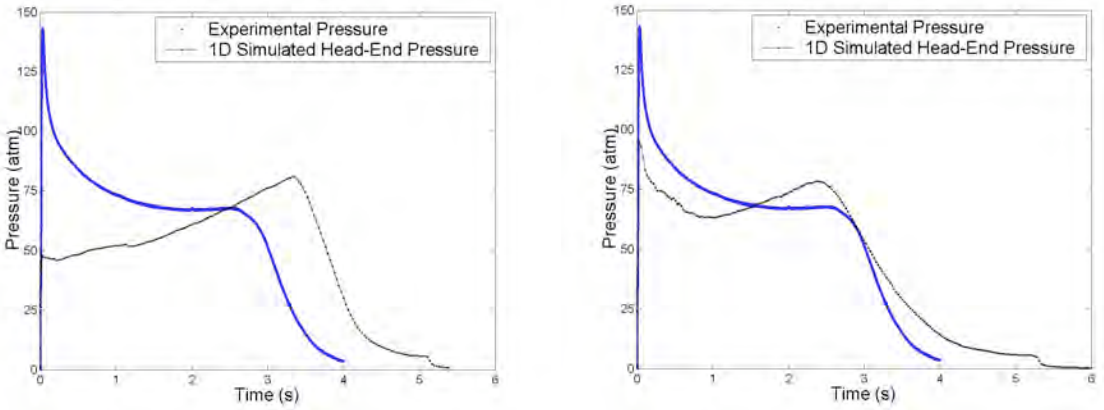

Fig. 3.2.16: NAWC Motor #6 head-end pressure history. (Left) without erosive burning, (right) with erosive burning.

be implemented. This allows reasonable accuracy in full burn RSRM simulation at quasi-steady burning stage with significantly reduced computer time by switching from three-dimensional flow simulation to *Rocgrain/Rocballist*.

Physical Modeling

Aluminum Combustion Modeling and Aluminum/Propellant Interactions (Krier, Aita, Glumac, and Vanka)

There is much debate about how ultra-fine aluminum particles aid in rocket performance. Before any definitive results can be determined, a more accurate numerical model must be developed. Previous models become less accurate as the particle size decreases (d<20μm), for this reason the current model takes into account the burning of nano-sized particles using a shrinking core formulation. The debate at this point includes the question of whether or not smaller particles release energy more rapidly.

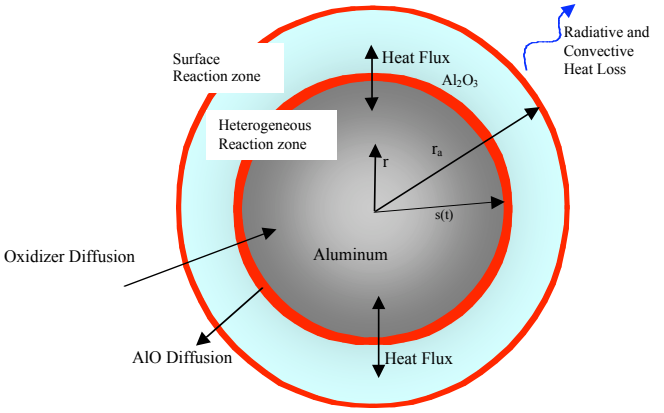

Figure 3.2.17: Combustion process schematic for nano-sized aluminum particle. In Model A: no surface reaction zone and no AlO diffusion. Model B: no oxidizer diffusion.

The shrinking core model, as seen schematically in Figure 3.2.17, is solved implicitly using a second-order finite differencing scheme. The equations of continuity and energy are solved with a moving boundary at the metal/oxide interface to find temperature history and burn time. The overall particle diameter is kept constant. The diffusion of reacting species through the oxide layer is the rate-limiting step. The first phase of the model, Model A, involves the diffusion of oxidizer towards the aluminum/oxide interface.

Figure 3.2.18 shows burn times for different concentrations of oxygen. The figure compares results determined by UIUC Shock Tube experiments and Model A. The figure shows the current model fits well for higher concentrations of oxidizer, while lower concentrations are yet to be predicted accurately by the model. Future work will be to modify the model to compensate for the high burn times at low oxidizer concentration.

Model A is currently being used to investigate burn time values and compare them to published experimental results in order to determine the limitations of the model. Future plans include developing the second phase of the model, Model B. This model includes the formation of AlO by reaction at the metal/oxide interface and the diffusion of this suboxide species to the surface. There is an additional reaction at the surface with ambient oxidizer. This mechanism, originally proposed by Doremus, is supported by experimental

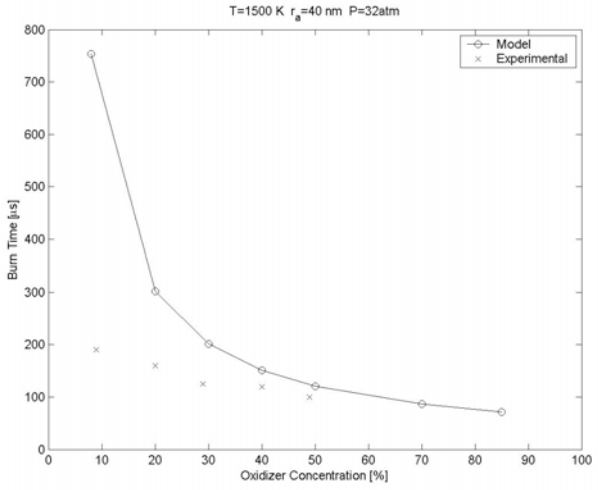

Fig. 3.2.18: Burn time as function of oxygen concentration using fit parameters found from Arrhenius plot. Experimental results are compared to model predictions.

results taken from Shock Tube experiments, in which AlO is seen to be present in a cloud of burning aluminum nano-particles.

The main issue that needs to be addressed in developing Model B is the uncertainty in the values for parameters defining chemical reaction and diffusion of AlO. This new area of aluminum powder combustion has many uncertainties that are similar to those mentioned previously, which makes it a difficult phenomenon to model.

In the third phase the two models will then be combined together. This third phase of the model will be used in several ongoing investigations such as:

- Ignition time and height of single nano-sized aluminum particles in fine AP
- Time resolved temperature history of aluminum convected off propellant surface
- Burn rate of propellant vs. pressure for different amount (%) of nano-sized aluminum

Curvature Effects in Solid Propellant Flames (Stewart, Kuznetzov, Yoo)

A small-curvature limit was used studied to determine curvature effects on deflagration of a curved surface of a homogeneous energetic material, i.e. a solid propellant. Under the assumption of quasi-steady deflagration, a method of matched asymptotics was employed to derive first order curvature corrections to the burning rate and surface temperature. As an illustration, a problem of spherical particle deflagration was solved numerically and compared successfully against the asymptotic solution. The underlying assumption of quasi-steady deflagration is verified by comparing results obtained for spherical particle deflagration to those obtained by a fully coupled unsteady solver. Corrections to planar formulas can be as large as 10 % and more. A study of the accuracy of interface-tracking algorithms and the inherent oscillations near the solid-gas interface that such algorithms produced was performed. For the important case when the surface regression rate depends on the high-activation-energy kinetics in the solid phase, the value of the mass flux is highly sensitive to even relatively small oscillations of the surface temperature. Sufficient accuracy was only achieved by computing in a frame fixed to the interface. A paper entitled, “Curvature effects in Solid Propellant Flames” is complete and being prepared for submission to *Combustion Theory and Modeling*.

Time Integration Methods for Solid Propellant Grain Burn Back – Theoretical Framework (Stewart, Brewster, and Tang)

This project is in conjunction with the Full Burnout project described above with Brewster, et al. Here we address the theoretical framework of the relative time-scaling problem. During the last year we consider the efficient computation of stable burn-back of a solid rocket motor when the motor is in a quasi-steady burning regime of operation. When the motor is modeled as a cavity that is filled with a compressible fluid with normal mass and momentum and energy injection from the solid propellant/gas interface; the problem posed is a standard one as a problem in steady computational aerodynamics. For large rockets such as the space shuttle solid rocket booster, the problem of quasi-steady solid rocket motor ballistic flow is analogous to the steady aerodynamic problem of flow past a large aircraft such as a Boeing 757 or F16 (say) flying at speeds such that compressible flow past the aircraft must be fully accounted for. One can wholly adopt the highly developed and advanced time integration strategies developed for application to commercial/military aircraft to the solid rocket motor grain burning to compute a series of realizations of steady flows as the grain burns back to near-completion. The slow regression of the solid propellant/gas interface is analogous to the motion of control surfaces on the aircraft as it moves through a controlled maneuver. Through the use of straightforward two-timing multi-scale asymptotic analysis we developed a reduced quasi-steady description of the quasi-steady burning regime for a model problem that is extensible to a full 3-D rocket.

Our first efforts studied a one-dimensional model of rocket combustion that employed the 1D compressible flow equations with area changes and mass sidewall injection that was state-dependent. We developed exact steady solutions for the configuration with frozen geometry and then time integrated the regression equations. We also implemented a multi-grid method as a typical fast solver for the steady flow and achieved the accelerated convergence rates similar to reported in the literature for these methods. A paper entitled, "Multi-scale modeling of solid rocket motors: time integration methods from computational aerodynamics applied to stable quasi-steady motor burning, D. Scott Stewart, K. C. Tang, Sunhee Yoo, Quinn Brewster and Igor Kuznetzov, was completed and submitted and is under consideration by the Journal of Propulsion and Power.

We worked late this spring and through the summer to develop the same methodologies for a two-dimensional axi-symmetric rocket configuration. In this regard we implemented a 2D Euler solver in AXS2D, coupled with our level set method used to represent the propellant grain interface. Thus we can easily test steady state relaxation of an Euler rocket model. In collaboration with Prof. Balachandar we started the implementation of a Newton, Kondratiev relaxation techniques to accelerate convergence of to a frozen steady state. At the end of the summer of 2005, Igor Kuznetzov departed CSAR to take a postdoctoral position at Boston University working with Micha Dembo modeling cell interfaces. This work is still underway.

Future Plans We will continue to work with Brewster, et al., on implement reduced models for grain burnback solid propellant design. We have just hired Pratik Bhatacharjee for the Fall 2005 semester to help us finish the NK relaxation study started with Igor Kuznetzov. We anticipate having 2D parametric relaxation study finished by the end of the Fall Term and plan to work with Balachandar. We also have worked with Brewster and his student to implement arbitrary 3D rockets shapes drawn by ProE, and important those grain shapes to our reduced models. These are described in the full burnout project section above. We also plan to collaboration with Dr. David Kassoy on the reduced asymptotics associated with rationally developed time zooming. This is developed from explicit asymptotics, as opposed to ad hoc modeling. We are also working with Balachandar and Hasselbacher on application of unsteady drag past particles and we are comparing results computed from *Rocflo* against those computed with the higher order AXS code.